



wwPDB EM Validation Summary Report ⓘ

Jul 6, 2026 – 10:39 PM JST

PDB ID : 9VU1 / pdb_00009vu1
EMDB ID : EMD-65349
Title : Structure of hTRPA1 complexed with LIQA
Authors : Min, Y.M.; Zonglin, D.Z.; Yang, Y.Y.
Deposited on : 2025-07-12
Resolution : 2.59 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

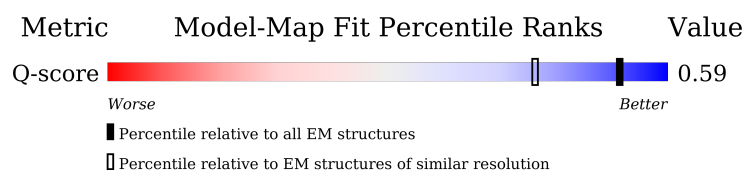
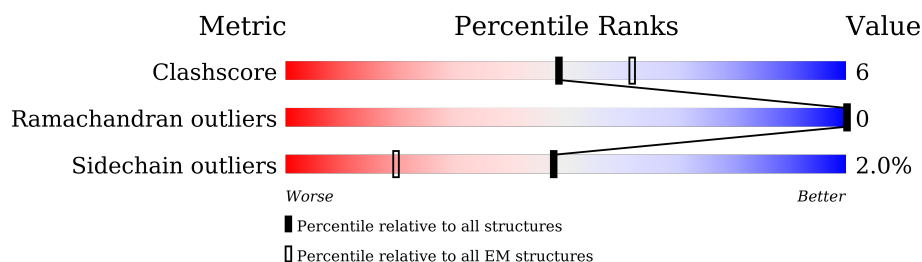
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

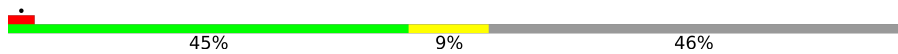
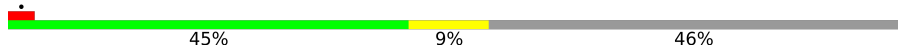
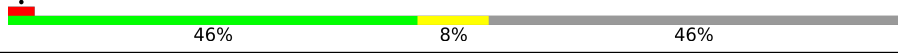
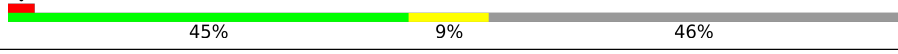
The reported resolution of this entry is 2.59 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7741 (2.09 - 3.09)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1119	
1	B	1119	
1	C	1119	
1	D	1119	

2 Entry composition [i](#)

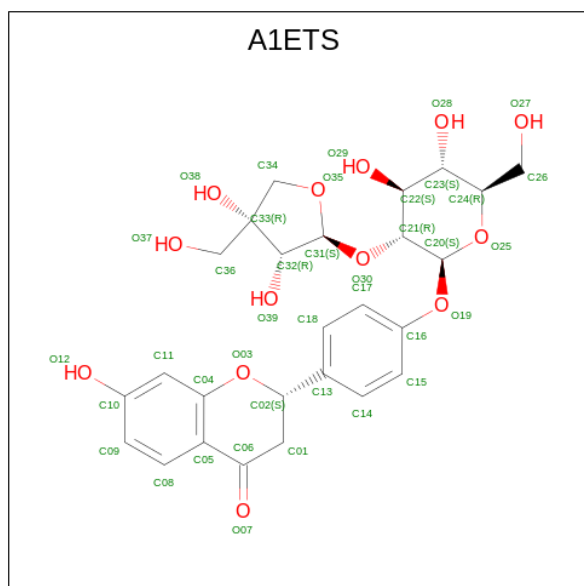
There are 2 unique types of molecules in this entry. The entry contains 19292 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Transient receptor potential cation channel subfamily A member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	605	Total	C	N	O	S	0	0
			4784	3138	786	823	37		
1	B	605	Total	C	N	O	S	0	0
			4784	3138	786	823	37		
1	C	605	Total	C	N	O	S	0	0
			4784	3138	786	823	37		
1	D	605	Total	C	N	O	S	0	0
			4784	3138	786	823	37		

- Molecule 2 is Liquiritin apioside (CCD ID: A1ETS) (formula: C₂₆H₃₀O₁₃) (labeled as "Ligand of Interest" by depositor).

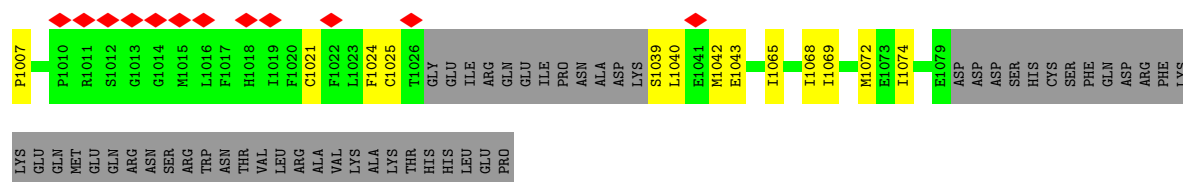


Mol	Chain	Residues	Atoms			AltConf
2	A	1	Total	C	O	0
			39	26	13	
2	B	1	Total	C	O	0
			39	26	13	

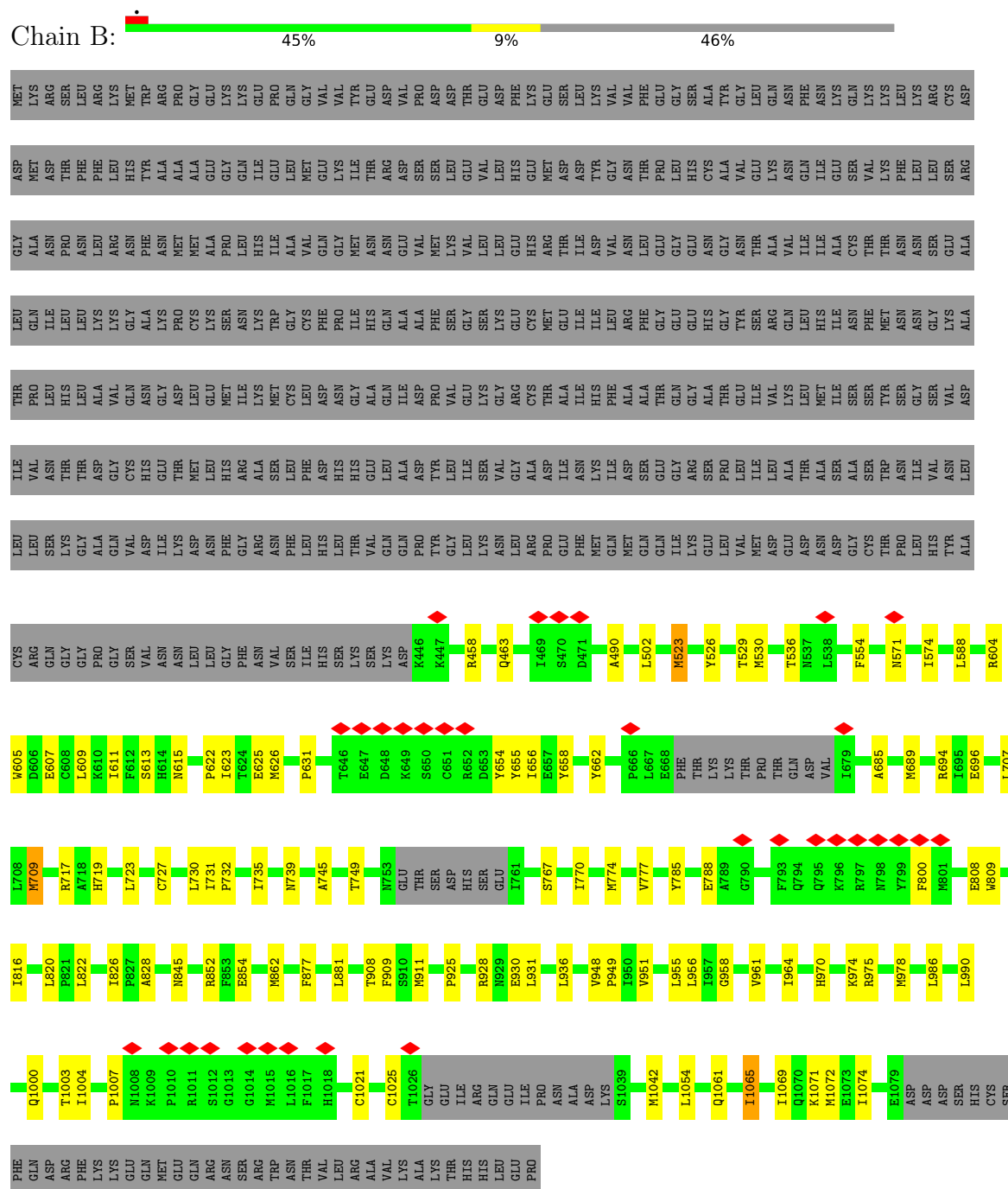
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Mol	Chain	Residues	Atoms			AltConf
2	C	1	Total	C	O	0
			39	26	13	
2	D	1	Total	C	O	0
			39	26	13	



- Molecule 1: Transient receptor potential cation channel subfamily A member 1



- Molecule 1: Transient receptor potential cation channel subfamily A member 1

ALA	GLU	L867	C727	N549	CYS	LEU	TLE	THR	LEU	GLN	GLY	ASP	MET
LYS	ILE					LEU	VAL	PRO	LEU	GLN	ALA	MET	LYS
THR	ARG	F877	L730	F554	ARG	SER	ASN	LEU	ASN	ILE	ASP	ASP	ARG
HIS	GLU					GLY	THR	HIS	LEU	LEU	ASN	THR	SER
LEU	ILE	T908	P732	N571	PRO	ALA	ASP	ALA	LEU	LYS	LEU	PHE	ARG
LEU	PRO				GLY	GLN	GLY	VAL	GLN	LYS	ARG	LEU	LYS
ASN	ASN	M911	I735	L588	SER	VAL	CYS	GLN	ASN	GLY	ASN	HIS	MET
ALA	ALA				VAL	ASN	HIS	ASN	TRP	ALA	PHE	TYR	ALA
ASP	ASP	P925	N739	R604	ASN	ILE	GLU	GLY	ASN	LYS	ALA	ASP	ARG
LYS	LYS				ASN	LYS	THR	THR	LYS	PRO	MET	ALA	PRO
S1039		R928	M744	N615	LEU	ASP	MET	LEU	CYS	CYS	MET	GLY	GLY
L1040		R929	A745		LEU	ASN	LEU	GLU	LYS	LYS	ALA	GLU	GLU
E1041		E930			GLY	PHE	HIS	MET	SER	PRO	ALA	GLU	LYS
M1042		L931	T749	M626	ASN	ARG	ALA	ILE	ASN	GLN	ILE	GLN	LYS
E1043					ASN	ASN	ALA	ALA	ILE	LYS	ILE	GLY	ILE
		L936	N753	P631	VAL	ASN	SER	MET	TRP	TRP	ILE	GLU	PRO
I1065			GLU		SER	PHE	LEU	CYS	GLY	CYS	ALA	LEU	GLY
		V948	THR		ILE	LEU	PHE	LEU	LEU	GLN	VAL	MET	GLY
I1068		P949	SER	T646	HIS	HIS	THR	ASP	ASN	PHE	GLN	GLU	VAL
I1069			ASP	E647	LYS	THR	HIS	GLY	ASN	PRO	GLY	LYS	GLY
Q1070		L955	HIS	D648	LYS	THR	HIS	GLY	ASN	ILE	MET	ILE	TYR
K1071		L956	GLU	K649	SER	VAL	GLU	ALA	ASN	HIS	ASN	THR	GLU
M1072		T957	SER		LYS	GLN	LEU	GLN	GLN	ALA	ASN	ARG	ASP
E1073		G958	GLU	S650	ASP	GLN	ALA	ILE	ALA	ALA	GLU	ASP	VAL
I1074			L762	C651		PRO	TYR	ASP	ASP	ALA	VAL	SER	PRO
		V961		R652	K446	GLY	THR	PRO	PHE	ASN	ASP	ASP	ASP
E1079			S767	D853	K447	LEU	ILE	GLU	SER	LYS	LYS	LEU	THR
ASP	ASP	I964	I770	Y654	L450	LYS	SER	LYS	SER	GLY	LEU	VAL	GLU
ASP	ASP	H970		I655	R458	ASN	VAL	GLY	ASN	LYS	LEU	VAL	ASP
SER	SER		M774	I656		LEU	GLY	ARG	GLU	GLY	GLU	HIS	PHE
HIS	HIS	K974		E657	Q463	ARG	ALA	CYS	CYS	HIS	GLY	GLU	LYS
CYS	CYS		V777	Y658		PRO	ASP	THR	MET	MET	ARG	MET	GLU
SER	SER	M978				GLU	ILE	ALA	GLU	GLU	THR	ASP	SER
PHE	PHE		E788	Y662	I469	PHE	ASN	ILE	ILE	ILE	ILE	ASP	LEU
GLN	GLN	R996	A789	P666	S470	MET	LYS	HIS	MET	ILE	ASP	TYR	LYS
ASP	ASP		G790	L667	D471	GLN	ILE	PHE	LEU	VAL	GLY	GLY	VAL
ARG	ARG	Q1000				MET	ASP	ALA	ASN	ARG	ASN	ASN	VAL
PHE	PHE			E668	L474	GLN	SER	THR	PHE	GLY	THR	THR	PHE
LYS	LYS	T1003	F793			GLN	GLU	THR	THR	GLU	PRO	GLY	GLY
LYS	LYS		Q794	THR	D479	ILE	GLY	GLN	GLU	GLU	GLY	HIS	SER
GLN	GLN	P1007	Q795	LYS	L480	LYS	ARG	GLY	GLY	GLU	ASN	CYS	TYR
MET	MET			THR		LEU	SER	ALA	ALA	HIS	ALA	ALA	ALA
GLU	GLU	P1010	R1011	PRO	A490	VAL	PRO	GLU	THR	TYR	GLY	VAL	LEU
GLN	GLN	S1012	N798	THR	L502	MET	ILE	ILE	ILE	SER			

[illegible]

ARG	PHE	LYS	GLU	GLN	MET	GLU	ARG	SER	ASN	TRP	ARG	THR	VAL	LEU	ARG	ALA	VAL	GLY	ILE	GLN	ARG	GLU	THR	LEU	PRO																						
I1004	P1007	K1008	I816	L820	P821	L822	I826	P827	A828	N845	E854	M862	F877	L881	T908	F909	S910	M911	P925	R928	N929	E930	L931	L936	V948	P949	L955	L956	S957	G958	V961	I964	K974	R975	N978	R996	Q1000	T1003									
R694	I695	E696	L707	L708	M709	R717	L723	C727	L730	I731	P732	I735	N739	M744	A745	T749	N753	GLU	THR	SER	ASP	HIS	SER	GLU	I761	S767	I770	M774	V777	Y785	E788	A789	G790	F793	Q794	Q795	K796	R797	N798	Y799	F800	M801					
I574	L588	R604	W605	D606	E607	L609	S613	R614	N615	C621	P622	I623	T624	E625	N626	P631	S645	T646	E647	D648	K649	S650	C651	R652	D653	Y654	Y655	Y658	Y662	P666	L667	E668	PHE	THR	LYS	LYS	THR	PRO	THR	GLN	ASP	VAL	I679	A685	N689		
CYS	ARG	GLN	GLY	PRO	GLY	SER	VAL	ASN	ASN	LEU	LEU	GLY	PHE	ASN	ASN	VAL	SER	ILE	HIS	SER	LYS	SER	GLN	ASP	K446	K447	L450	R458	Q463	I469	S470	D471	L474	L480	A490	L502	M523	Y526	T529	M530	T536	M537	L538	F554	N571		
LEU	LEU	SER	LYS	ALA	GLN	VAL	ASP	ILE	LYS	THR	ASP	ASN	PHE	GLY	ARG	ALA	VAL	ASN	ASN	LEU	HIS	LEU	THR	VAL	GLN	ALA	PRO	TYR	GLY	LEU	ILE	LYS	ASN	VAL	GLY	ARG	GLU	SER	PRO	LEU	VAL	MET	THR	ALA	ASP	ASN	ALA
THR	PRO	LEU	THR	ASP	ALA	GLN	VAL	THR	ASP	LEU	LEU	PHE	HIS	ASP	HIS	HIS	GLY	LEU	VAL	GLN	GLN	ALA	ILE	ASP	PRO	TYR	VAL	GLY	LEU	ILE	ASN	VAL	GLY	ARG	GLU	SER	PRO	LEU	VAL	ASP	ASN	VAL	ASN	VAL	ASP	ALA	
LEU	GLN	ILE	LEU	LYS	LYS	GLY	LYS	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	106614	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.494	Depositor
Minimum map value	-0.952	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.14	Depositor
Map size ($\text{\AA}$)	307.04, 307.04, 307.04	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.808, 0.808, 0.808	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: A1ETS

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.10	0/4893	0.25	0/6632
1	B	0.10	0/4893	0.24	0/6632
1	C	0.10	0/4893	0.29	2/6632 (0.0%)
1	D	0.10	0/4893	0.23	0/6632
All	All	0.10	0/19572	0.26	2/26528 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1020	PHE	CA-C-N	-8.45	108.92	122.95
1	C	1020	PHE	C-N-CA	-8.45	108.92	122.95

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4784	0	4821	59	0
1	B	4784	0	4821	62	0
1	C	4784	0	4821	58	0
1	D	4784	0	4821	62	0
2	A	39	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	39	0	0	1	0
2	C	39	0	0	1	0
2	D	39	0	0	2	0
All	All	19292	0	19284	222	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 222 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1021:CYS:HB2	1:A:1025:CYS:H	1.23	1.02
1:C:1021:CYS:HB2	1:C:1025:CYS:H	1.39	0.88
1:A:458:ARG:NH2	1:C:1072:MET:O	2.24	0.70
1:A:1072:MET:O	1:D:458:ARG:NH2	2.25	0.69
1:A:709:MET:HE3	1:A:1000:GLN:H	1.58	0.69

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	597/1119 (53%)	579 (97%)	18 (3%)	0	100	100
1	B	597/1119 (53%)	578 (97%)	19 (3%)	0	100	100
1	C	597/1119 (53%)	570 (96%)	27 (4%)	0	100	100
1	D	597/1119 (53%)	572 (96%)	25 (4%)	0	100	100
All	All	2388/4476 (53%)	2299 (96%)	89 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	514/995 (52%)	502 (98%)	12 (2%)	44	71
1	B	514/995 (52%)	502 (98%)	12 (2%)	44	71
1	C	514/995 (52%)	505 (98%)	9 (2%)	51	76
1	D	514/995 (52%)	505 (98%)	9 (2%)	51	76
All	All	2056/3980 (52%)	2014 (98%)	42 (2%)	48	74

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	723	LEU
1	D	523	MET
1	C	744	MET
1	C	970	HIS
1	D	615	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	590	ASN
1	C	855	ASN
1	C	831	GLN
1	C	893	ASN
1	A	893	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	A1ETS	D	1201	-	43,43,43	3.36	9 (20%)	60,64,64	1.55	12 (20%)
2	A1ETS	B	1201	-	43,43,43	3.42	10 (23%)	60,64,64	1.54	11 (18%)
2	A1ETS	A	1201	-	43,43,43	3.41	10 (23%)	60,64,64	1.56	11 (18%)
2	A1ETS	C	1201	-	43,43,43	3.40	10 (23%)	60,64,64	1.54	10 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A1ETS	D	1201	-	-	10/17/65/65	0/5/5/5
2	A1ETS	B	1201	-	-	14/17/65/65	0/5/5/5
2	A1ETS	A	1201	-	-	14/17/65/65	0/5/5/5
2	A1ETS	C	1201	-	-	14/17/65/65	0/5/5/5

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1201	A1ETS	C34-C33	12.95	1.68	1.52
2	A	1201	A1ETS	C34-C33	12.86	1.67	1.52
2	B	1201	A1ETS	C34-C33	12.83	1.67	1.52
2	D	1201	A1ETS	C34-C33	12.11	1.67	1.52
2	B	1201	A1ETS	O03-C04	10.52	1.52	1.38

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	A1ETS	C16-O19-C20	-5.56	109.64	117.79
2	C	1201	A1ETS	C16-O19-C20	-5.49	109.75	117.79
2	B	1201	A1ETS	C16-O19-C20	-5.42	109.84	117.79
2	D	1201	A1ETS	C16-O19-C20	-4.60	111.05	117.79
2	A	1201	A1ETS	C20-C21-C22	3.77	116.87	110.38

There are no chirality outliers.

5 of 52 torsion outliers are listed below:

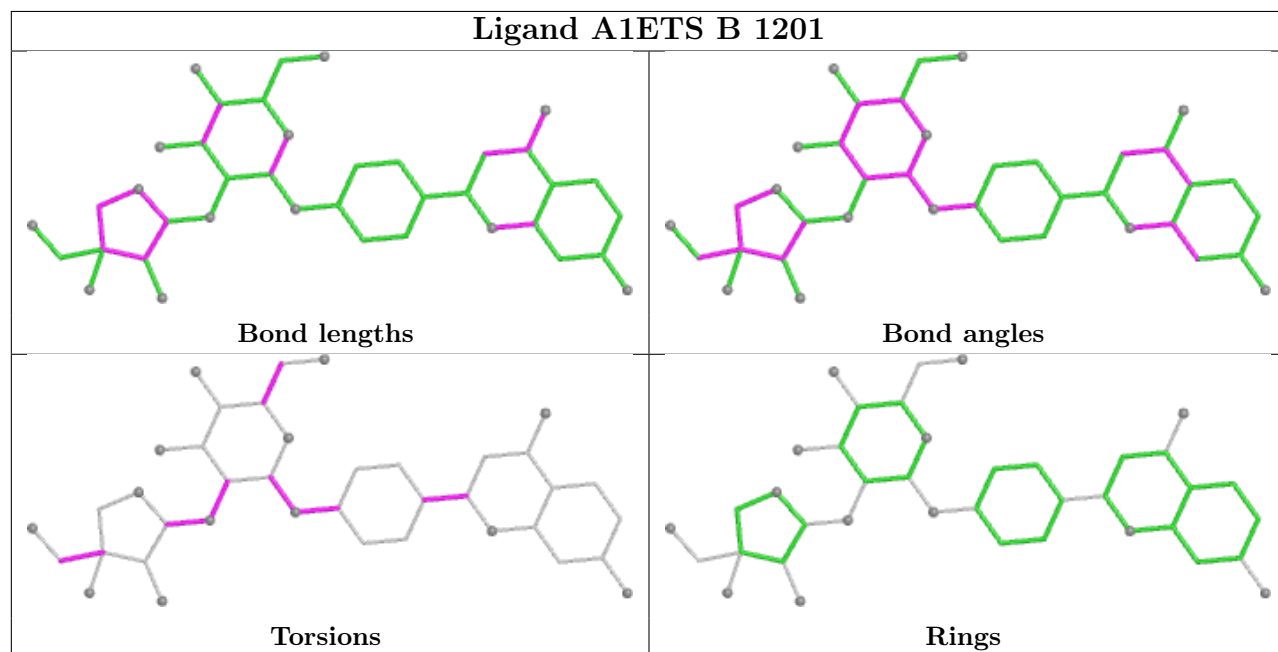
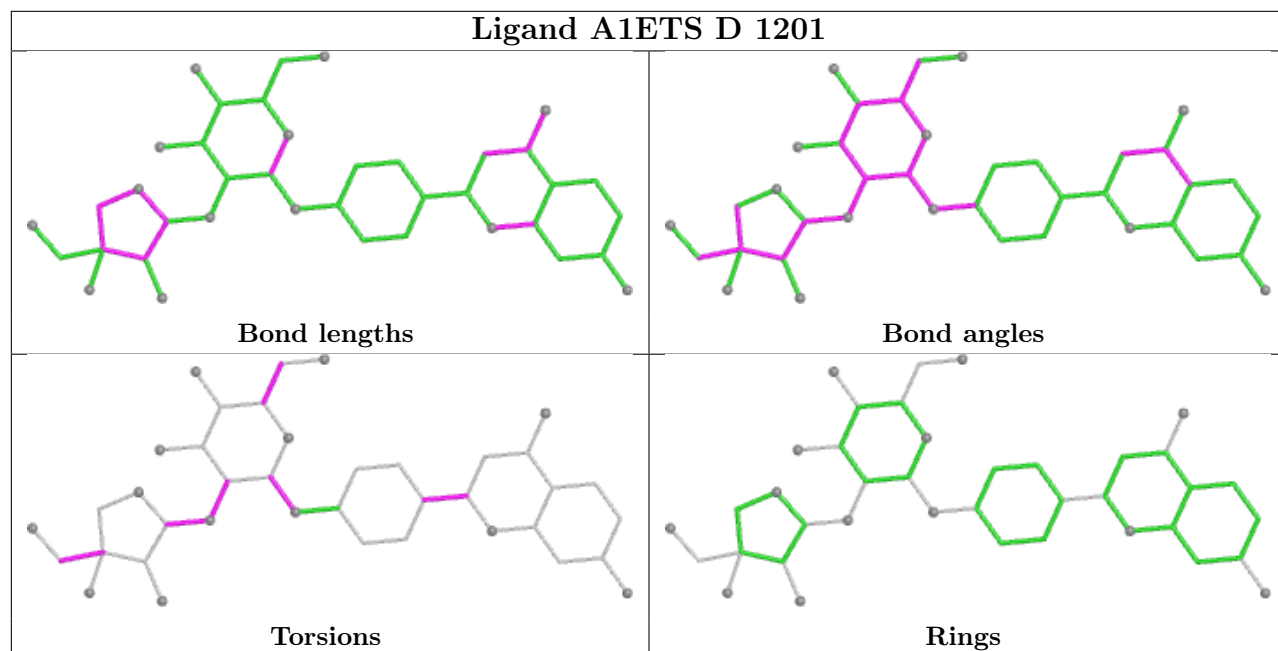
Mol	Chain	Res	Type	Atoms
2	A	1201	A1ETS	C20-C21-O30-C31
2	A	1201	A1ETS	O35-C31-O30-C21
2	A	1201	A1ETS	C32-C31-O30-C21
2	A	1201	A1ETS	O38-C33-C36-O37
2	A	1201	A1ETS	C34-C33-C36-O37

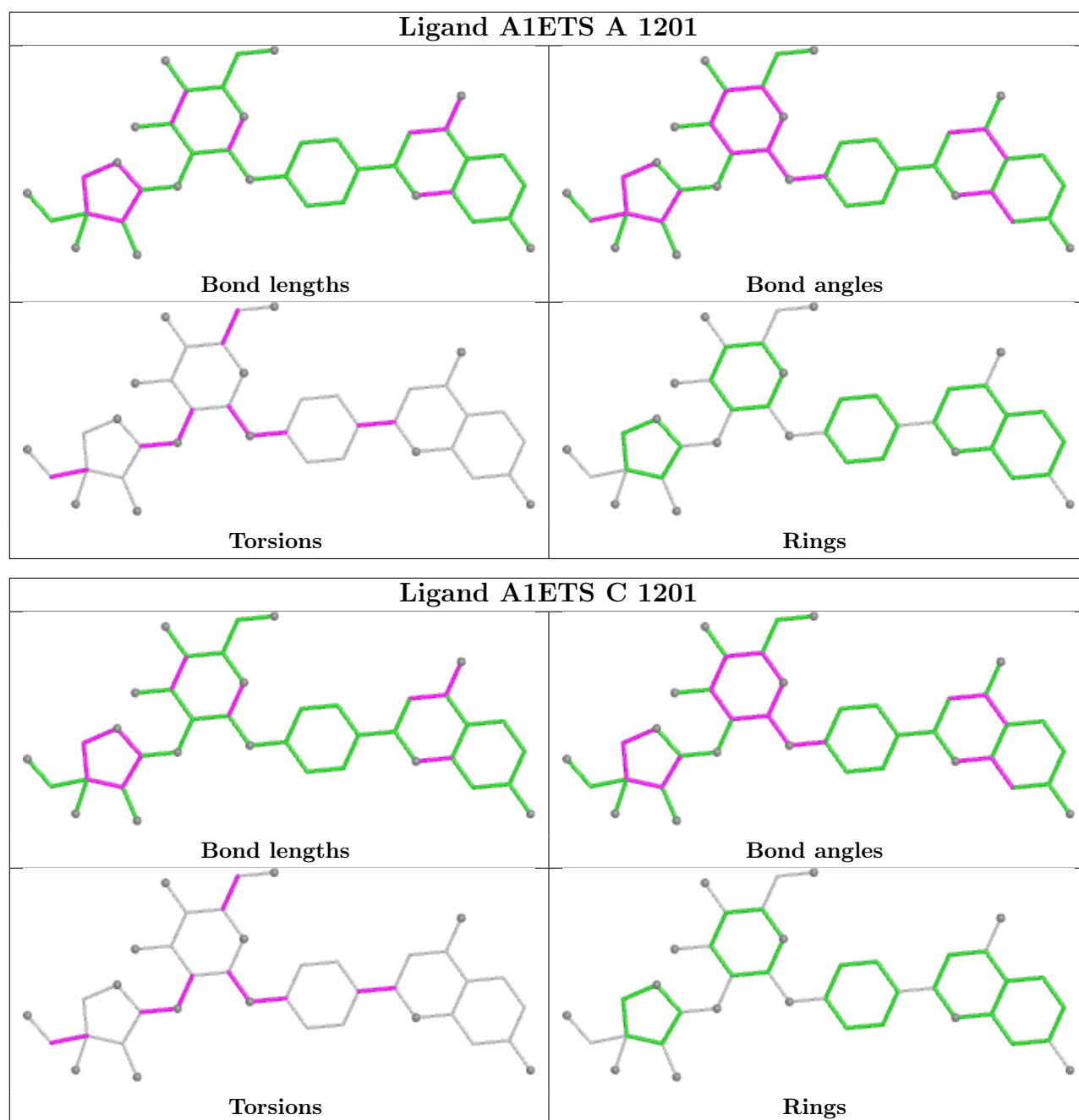
There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1201	A1ETS	2	0
2	B	1201	A1ETS	1	0
2	A	1201	A1ETS	1	0
2	C	1201	A1ETS	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

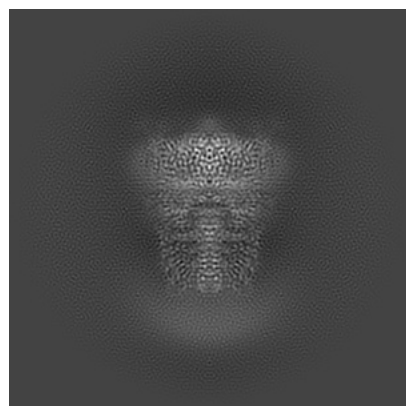
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65349. These allow visual inspection of the internal detail of the map and identification of artifacts.

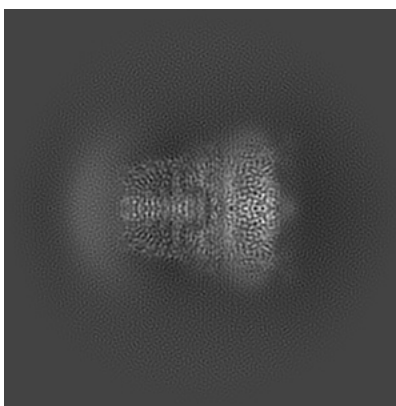
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

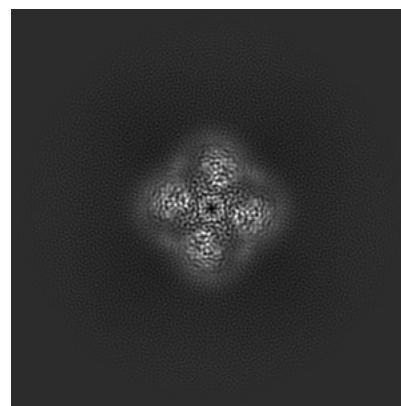
6.1.1 Primary map



X

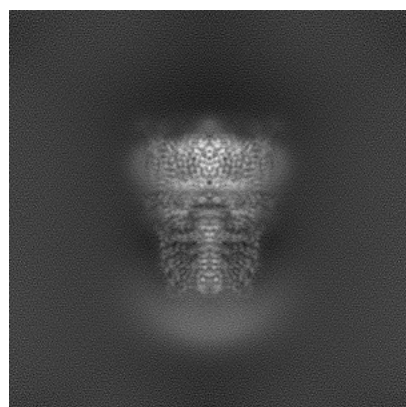


Y

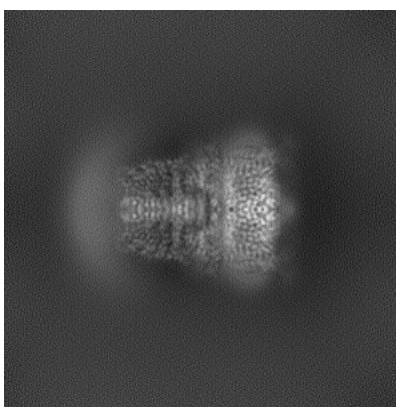


Z

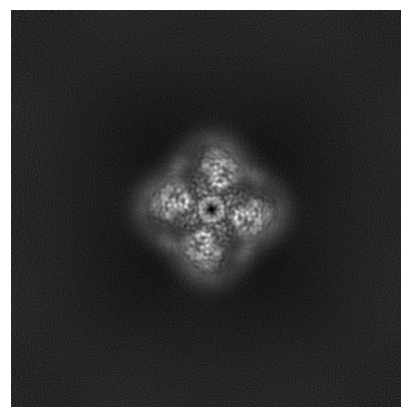
6.1.2 Raw map



X



Y

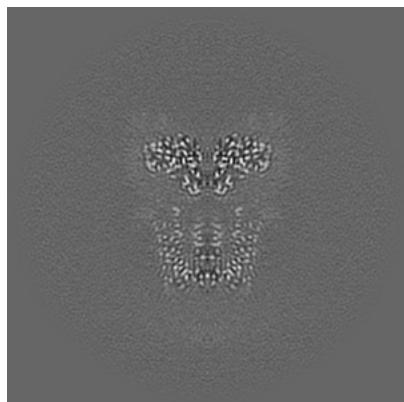


Z

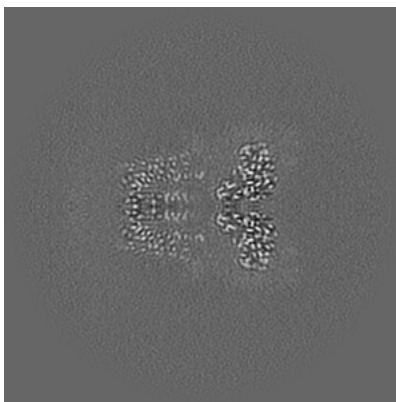
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

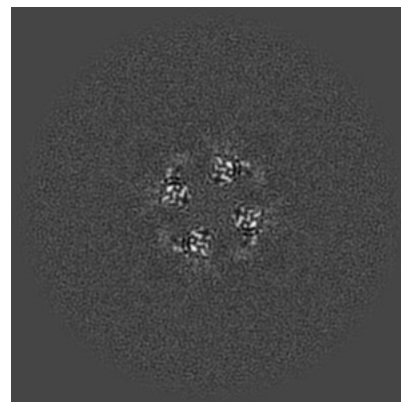
6.2.1 Primary map



X Index: 190

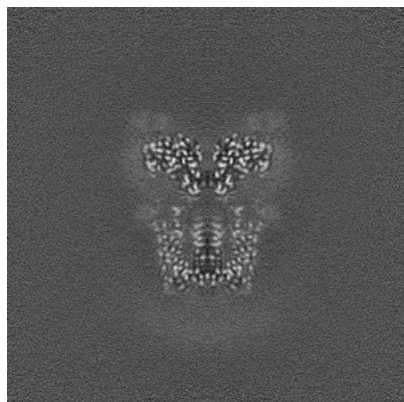


Y Index: 190

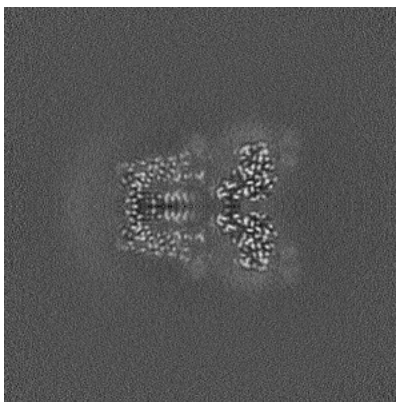


Z Index: 190

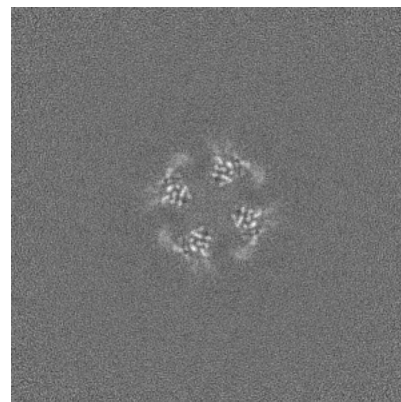
6.2.2 Raw map



X Index: 190



Y Index: 190

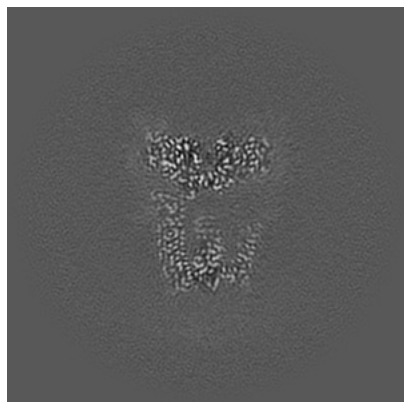


Z Index: 190

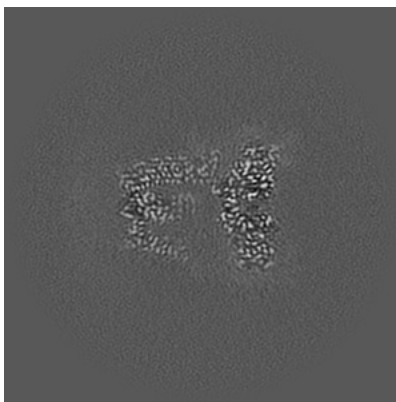
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

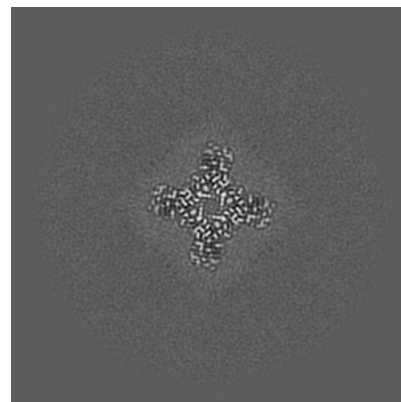
6.3.1 Primary map



X Index: 186

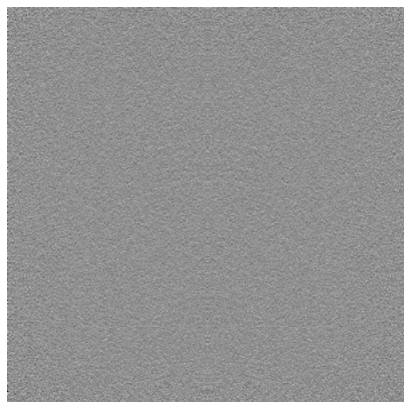


Y Index: 186

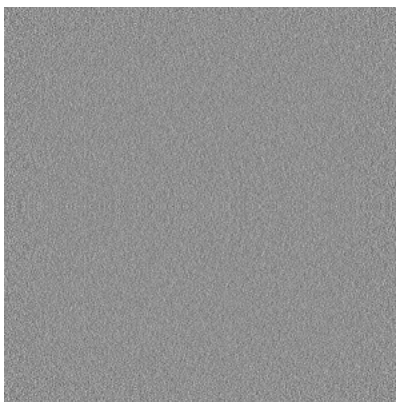


Z Index: 245

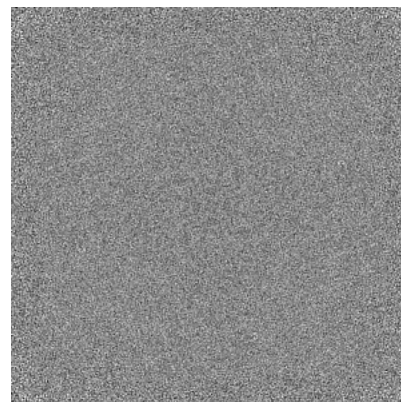
6.3.2 Raw map



X Index: 0



Y Index: 0

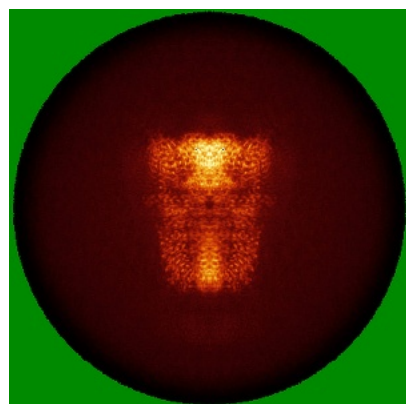


Z Index: 0

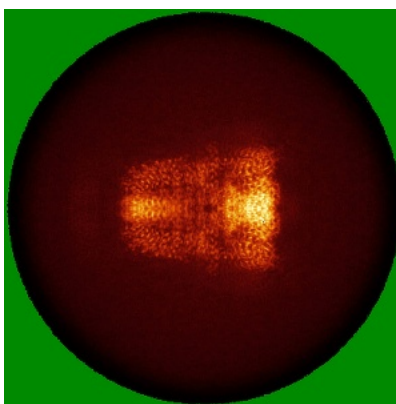
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

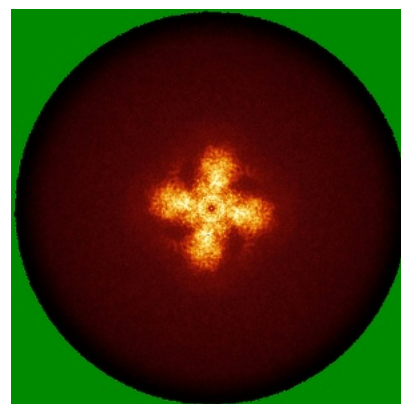
6.4.1 Primary map



X

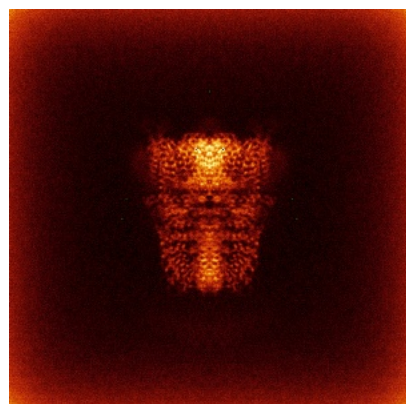


Y

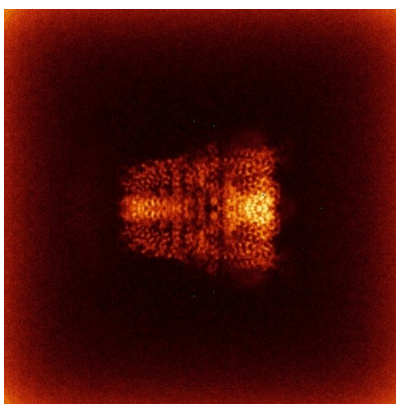


Z

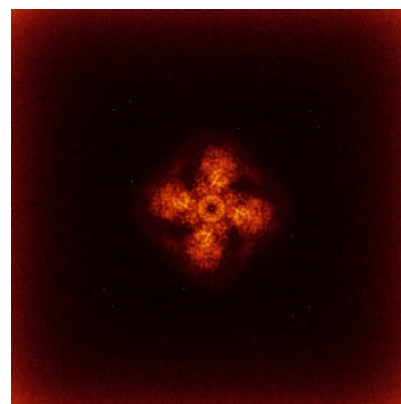
6.4.2 Raw map



X



Y

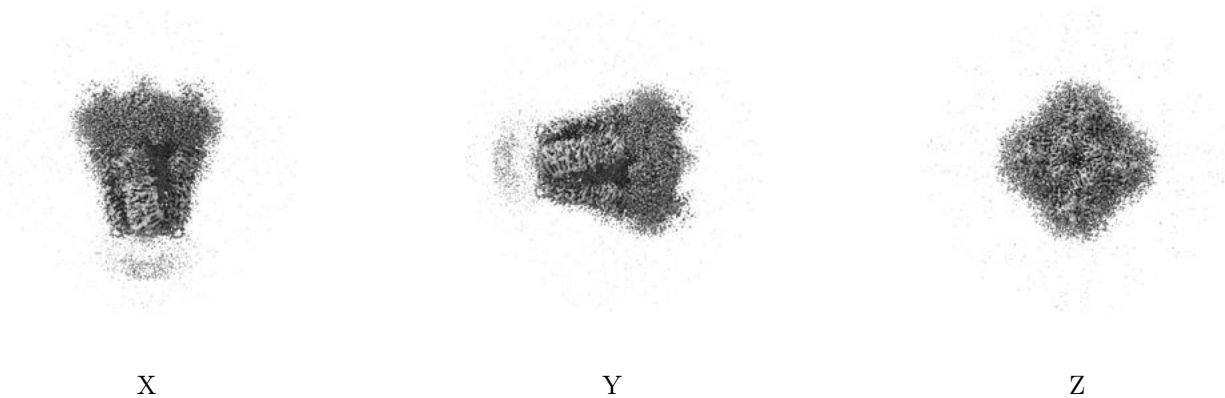


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

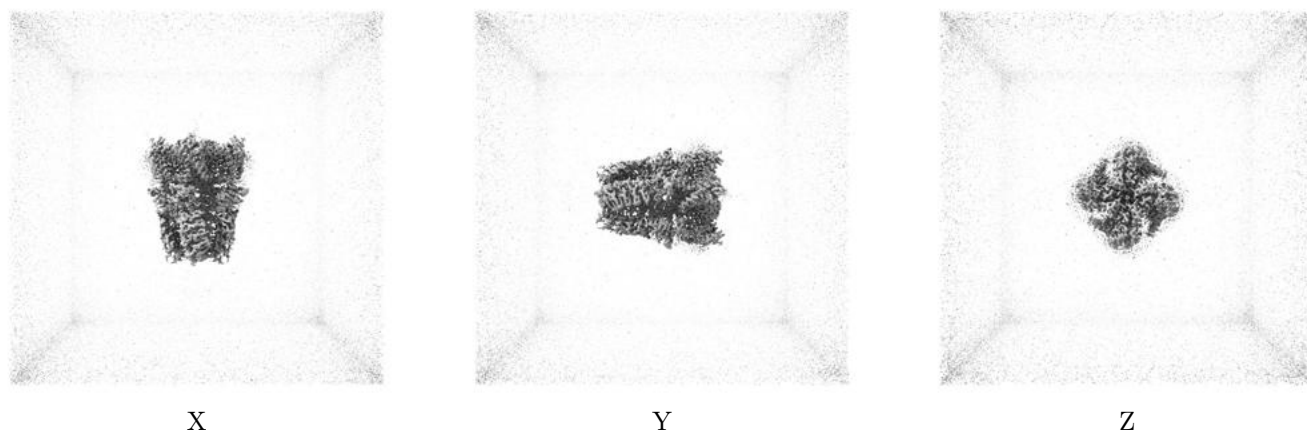
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.14. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

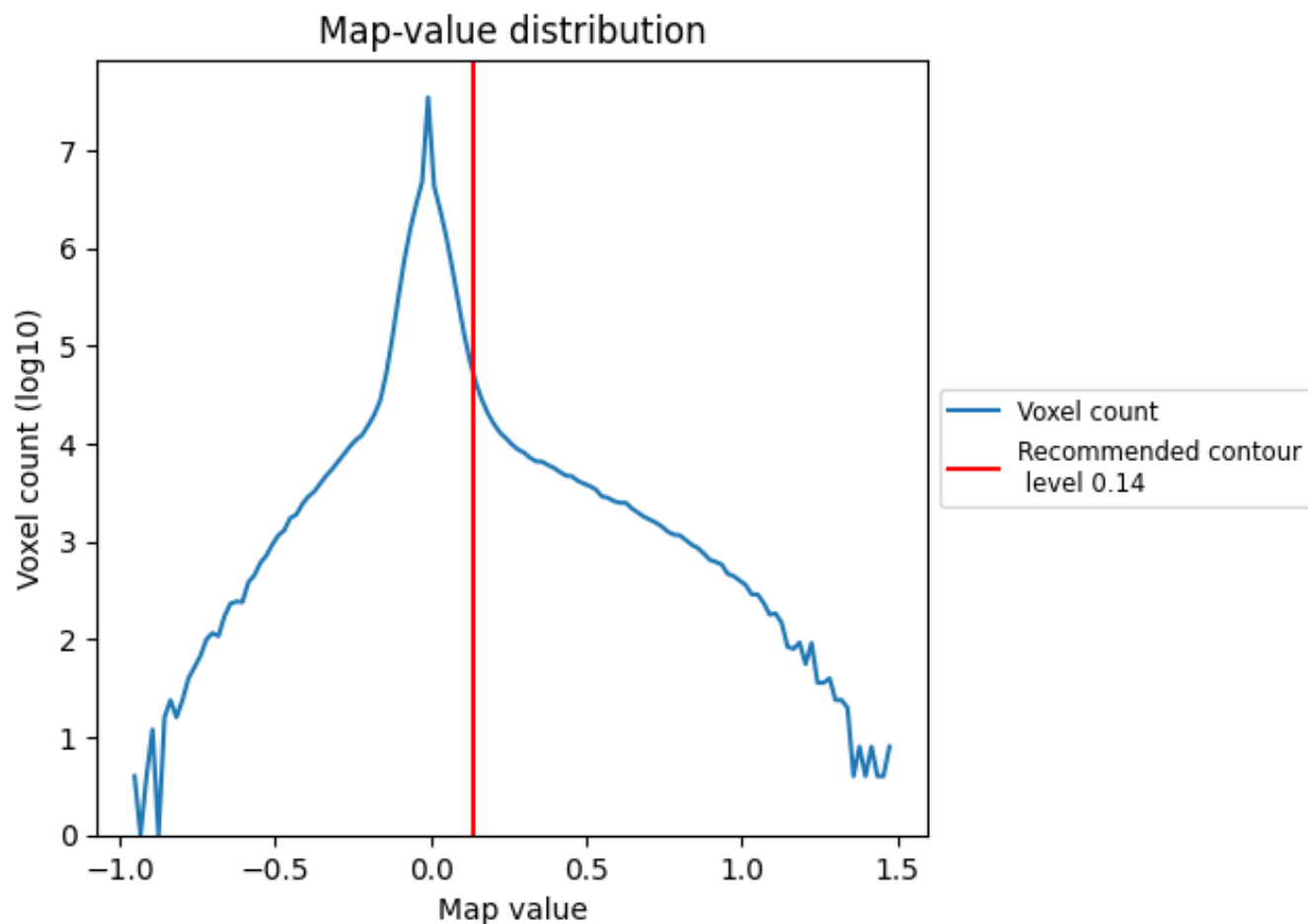
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

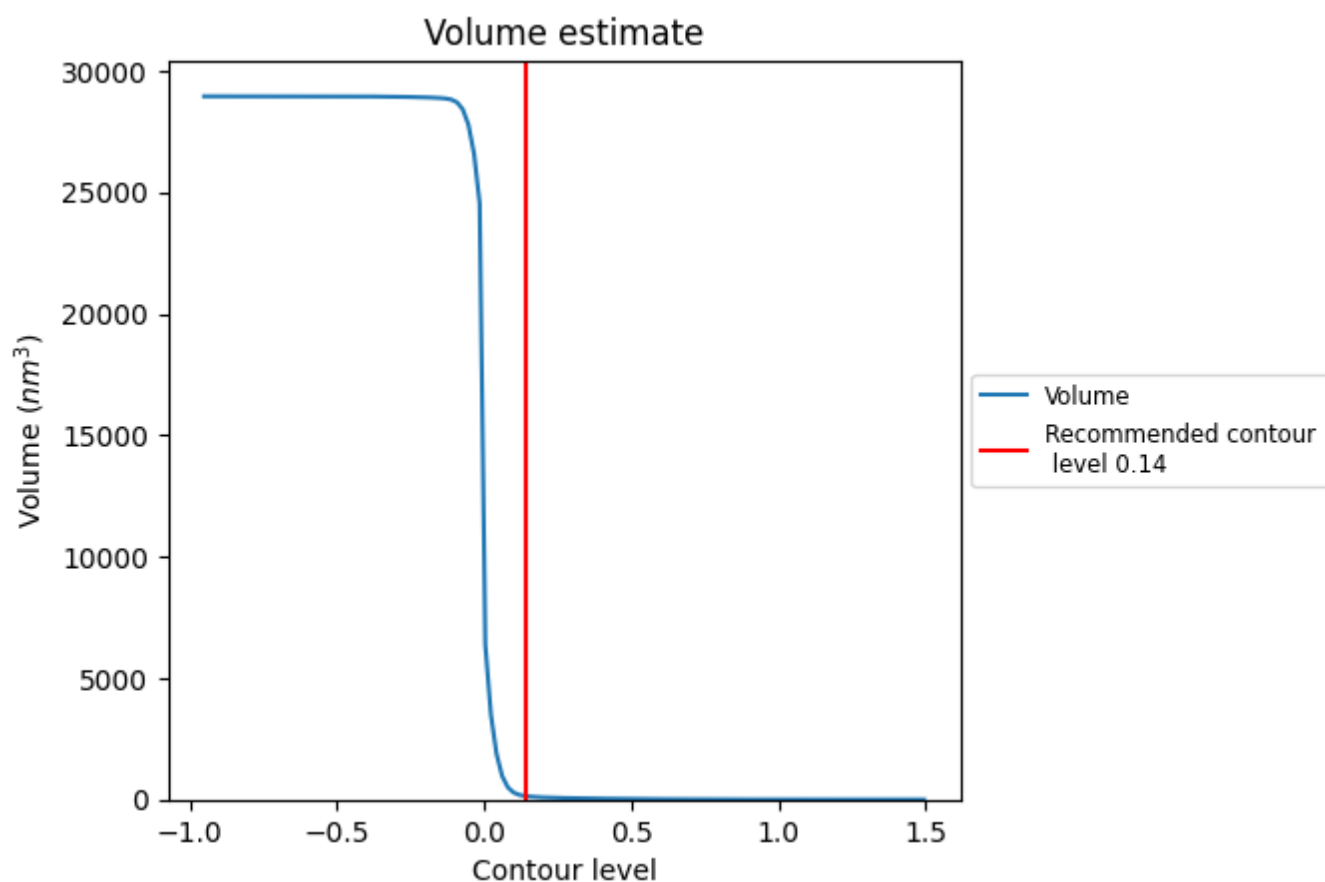
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

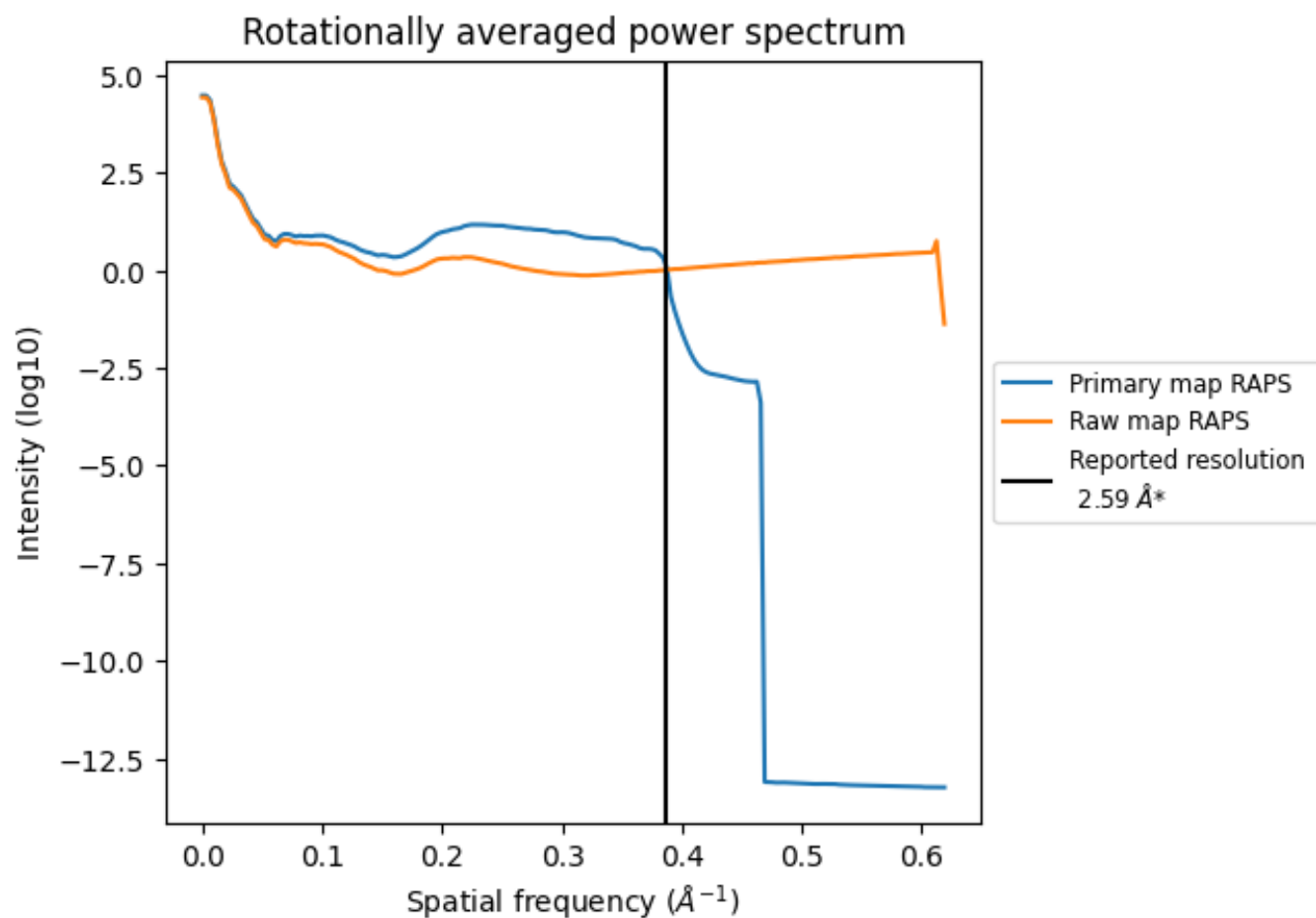
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 144 nm³; this corresponds to an approximate mass of 130 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

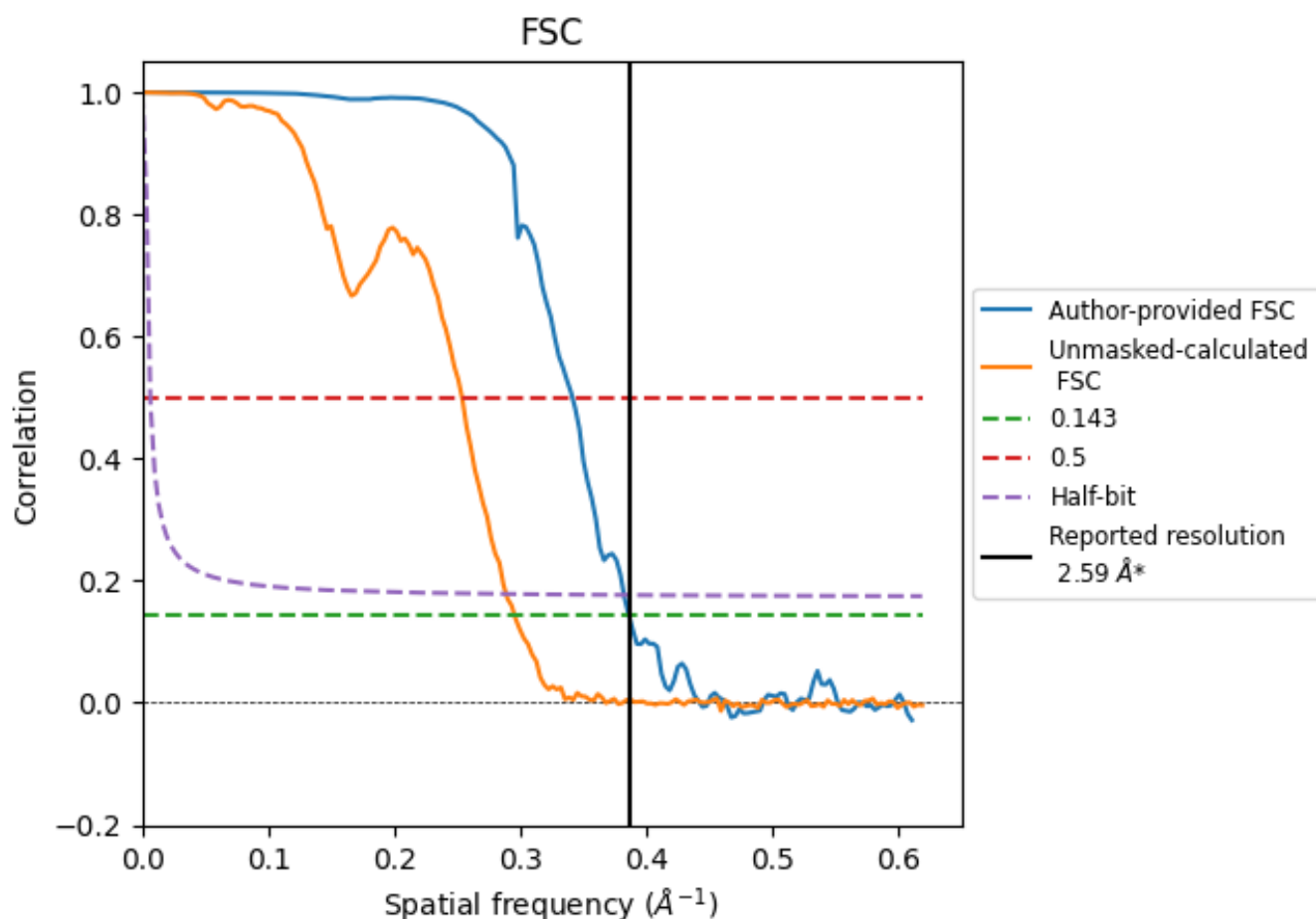


*Reported resolution corresponds to spatial frequency of 0.386 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.386 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

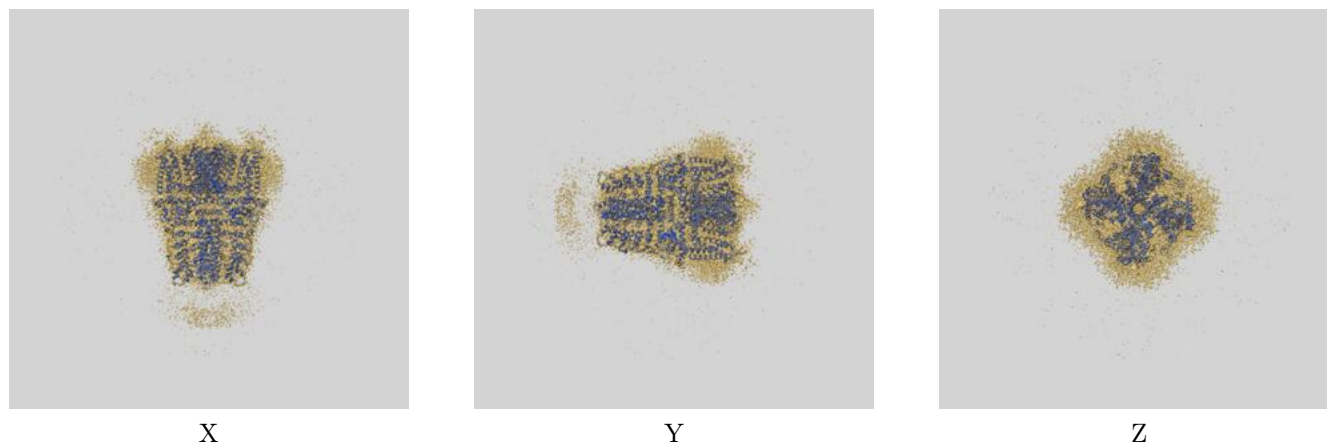
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.59	-	-
Author-provided FSC curve	2.59	2.93	2.62
Unmasked-calculated*	3.38	3.94	3.46

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.38 differs from the reported value 2.59 by more than 10 %

9 Map-model fit [i](#)

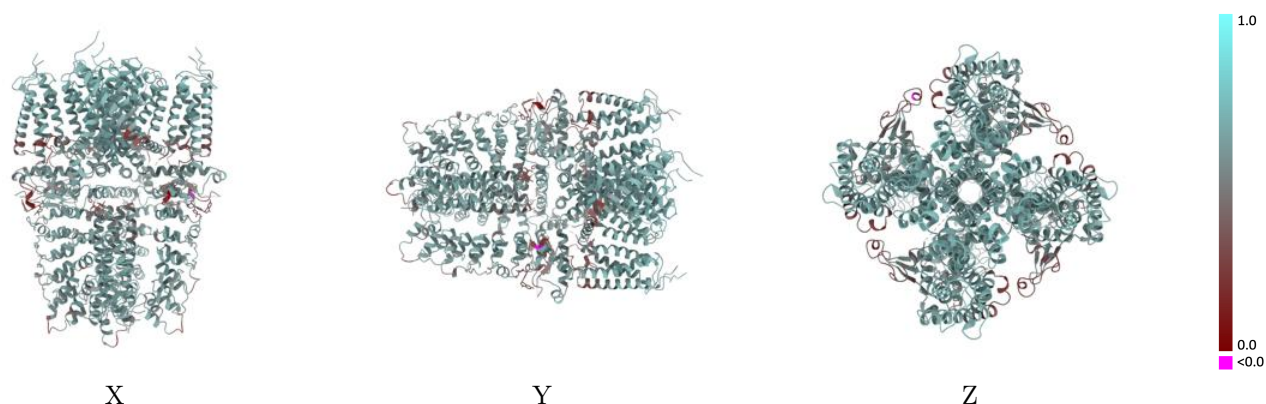
This section contains information regarding the fit between EMDB map EMD-65349 and PDB model 9VU1. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



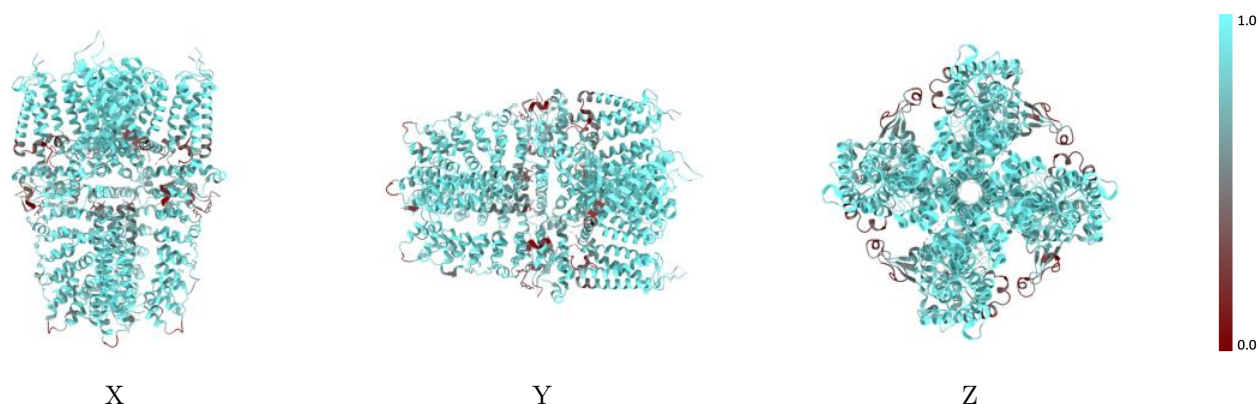
The images above show the 3D surface view of the map at the recommended contour level 0.14 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



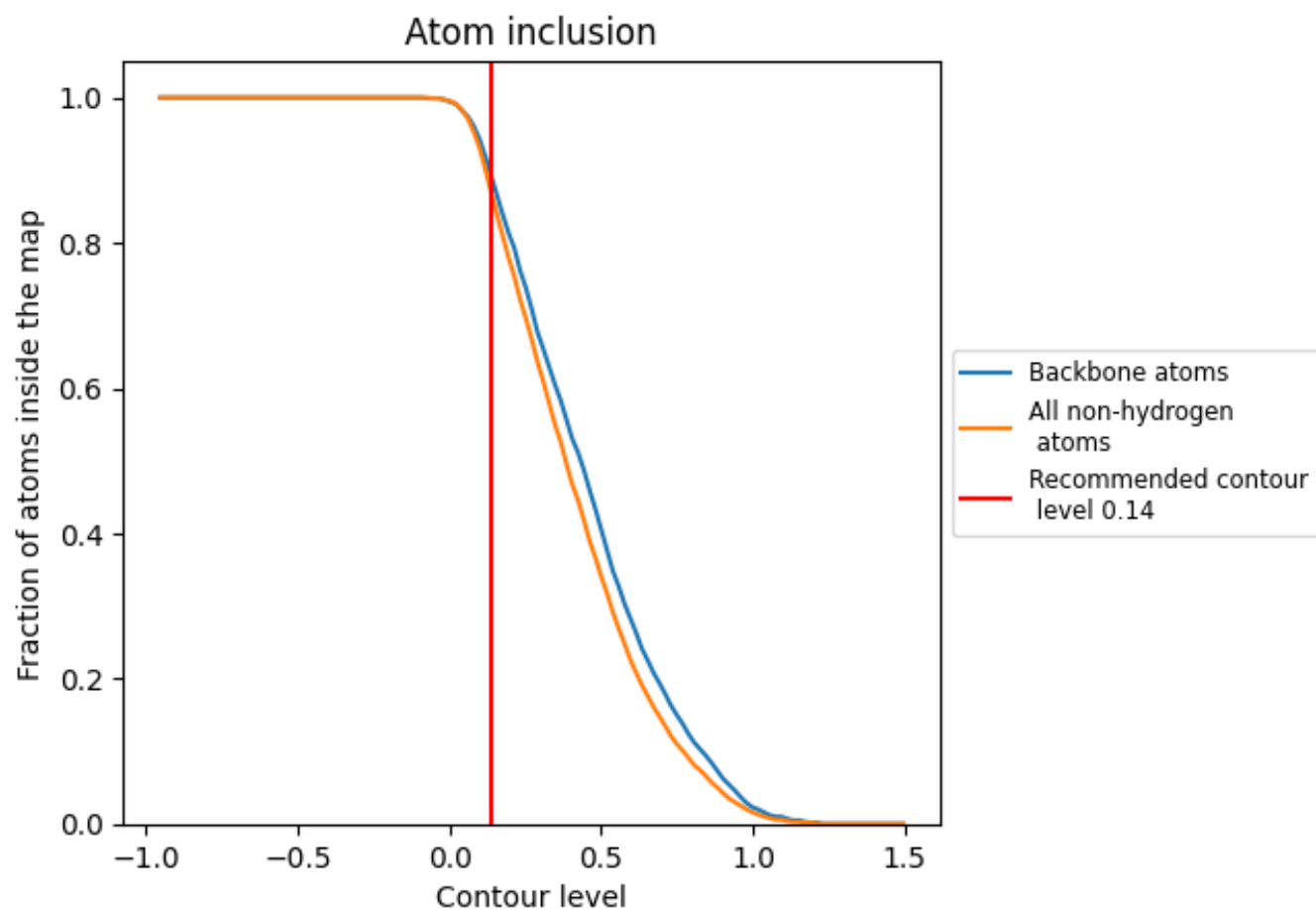
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.14).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.14) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8650	0.5900
A	0.8650	0.5890
B	0.8660	0.5910
C	0.8660	0.5900
D	0.8650	0.5910

